Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.76e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.38e-01

Confidence level: 2.93e-01

Nearest Neighbors from the Training Set

Image not found
Benz(a)anthracene
Measured: 1.97e-10
Predicted: 2.14e-08

Image not found
L-Glutamic acid
Measured: 1.70e-08
Predicted: 1.68e-08

Image not found
1,4-Benzenediamine, N-(2,4-dinitrophenyl)-
Measured: 3.28e-08
Predicted: 5.92e-11

Image not found
Lepidine
Measured: 8.02e-14
Predicted: 9.90e-03

Image not found
2,2,5,5-Tetramethylhexane
Measured: 9.80e-08
Predicted: 7.94